Equivalence of two Non–Equilibrium Ensembles via Propagation of Chaos

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Project funded by ANR SINEQ

SMAI 2025: Echantillonnage et métastabilité II

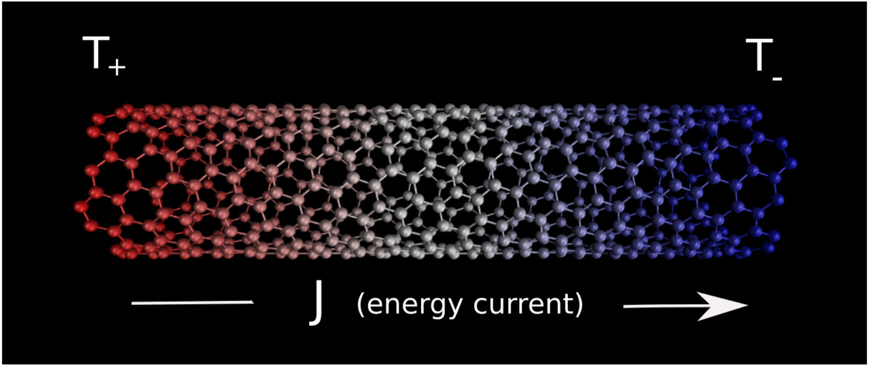
Outline

- **Two NEMD Frameworks**
  - Standard Fixed Forcing NEMD Framework (Thévenin Ensemble)
  - Fixed Response NEMD Framework (Norton Ensemble)
- **Mean–Field Interacting Particle Systems**
  - Setup and Standard Results
  - Norton Mean–Field System
  - Norton McKean–Vlasov Dynamics
- **Propagation of Chaos and Equivalence of Ensembles**
  - Propagation of Chaos for the Norton Dynamics
  - Equivalence of Ensembles from Propagation of Chaos
- **Extensions and perspectives**

(Non–)Equilibrium Molecular Dynamics

Steady–State Out–of–Equilibrium Systems

An external forcing on/perturbation of an equilibrium system induces a response



Here we are interested in the steady–state/long–time behavior.
Keyword: *Non–equilibrium steady state (NESS)*

Equilibrium Molecular Dynamics

Reference/Equilibrium dynamics on $\mathbb{R}^D$

$$dX_t^0 = b\left(X_t^0\right)dt + \sqrt{\frac{2}{\beta}}dW_t,$$

with (equilibrium) invariant probability measure ν_0.

Archetypal example: *Overdamped Langevin dynamics*

$$b\left(x\right) = -\nabla U(x), \qquad \nu_0(dx) \propto \mathrm{e}^{-\beta U(x)}dx$$

Remark: Overdamped dynamics is reversible with respect to its equilibrium measure.

Non–Equilibrium Molecular Dynamics

Perturb the reference dynamics by some external field F

Example: Perturb overdamped dynamics,

$$b\,(x) = -\nabla U(x), \qquad \nu_0(dx) \propto \mathrm{e}^{-\beta U(x)} dx,$$

with non–gradient external field F, i.e.

$$\nexists V : \mathbb{R}^D \to \mathbb{R}, \text{ s.t. } F = \nabla V.$$

Dynamics no longer reversible with respect to its invariant probability measure.

Question: *Force with what magnitude?*

Fixed Forcing NEMD (Thévenin Ensemble)

Dynamics perturbed by forcing of fixed magnitude $\eta \in \mathbb{R}$

$$dX_t^\eta = \left(b\left(X_t^\eta\right) + \eta F\left(X_t^\eta\right)\right) dt + \sqrt{\frac{2}{\beta}} dW_t,$$

with (non–equilibrium) invariant probability measure ν_η

For a given observable $R : \mathbb{R}^D \to \mathbb{R}$, measure response r

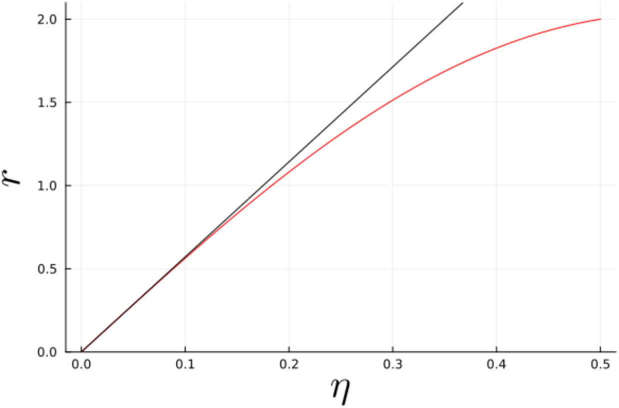
$$\mathbb{E}_{\nu_\eta}\left[R\left(X_t^\eta\right)\right] = \nu_\eta(R) = r(\eta)$$

Idea:

Fixing Forcing Magnitude		Measure Response
η	$\Longrightarrow$	$r(\eta) := \nu_\eta(R)$

Duality between η and r

One would expect a duality between the forcing magnitude and response—each η (locally) corresponds to a specific response $r(\eta)$



So we not fix the response r?

Fixed Response NEMD (Norton Ensemble)

Given an observable R and external force field F

Response fixed to $r \in \mathbb{R}$ by external forcing of variable magnitude:

$$\begin{cases} dY_t^r = b(Y_t^r)dt + \sqrt{\frac{2}{\beta}}dW_t + F\left(Y_t^r\right)d\Lambda_t^r \\ \Lambda^r \ : \mathbb{R}\text{–valued semi martingale fixing } R\left(Y_t^r\right) = r \end{cases}$$

Idea: Measure the forcing necessary to fix the response

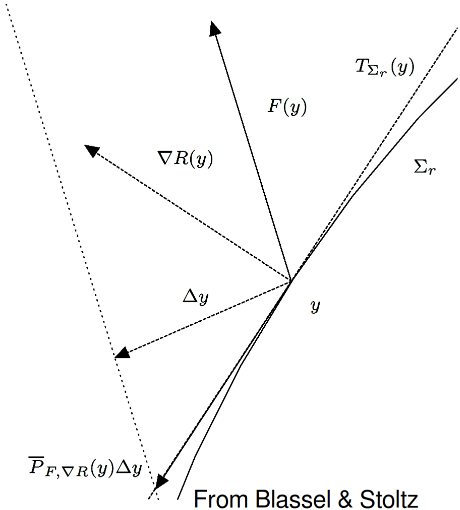
$$\begin{array}{ccc} \text{Fix Response} & & \text{Measure Response} \\ & \Longrightarrow & \\ r & & \text{"}\mathbb{E}\left[d\Lambda_t^r\right]\text{"} \end{array}$$

D.J. Evans, W.G. Hoover, B.H. Failor, B. Moran, and A.J.C. Ladd (1983) *Nonequilibrium molecular dynamics via Gauss's principle of least constraint.*

N. Blassel and G. Stoltz (2024) *Fixing the Flux: A Dual Approach to Computing Transport Coefficients*

Fixed Response NEMD (Norton Ensemble)

$F\left(Y_t^r\right) d\Lambda_t^r$ oblique projection onto $\Sigma_r = \left\{x \in \mathbb{R}^D : \; R(x) = r\right\}$
Λ^r a Lagrange multiplier



Equivalence of Fixed Response and Fixed Forcing NEMD?

Question: *Are these two descriptions equivalent?*

For fixed system and size, no!

Equivalence in some large particle limit like equilibrium equivalence of ensembles?

Equivalence of NVT and NVE ensembles

Local observable ϕ and conjugate inverse temperature β and energy E

$$\langle \phi \rangle^{\text{canonical}}_{\beta,N} \approx \langle \phi \rangle^{\text{microcanonical}}_{E,N}, \qquad \text{as } N \to \infty$$

Physicists say yes, but with a proof *à la physicienne*[1]

What can we prove rigourously (in a model case)?

[1] D.J. Evans (1993) *The equivalence of Norton and Thévenin ensembles*

Mean–Field Interacting Particle Systems

Thévenin Mean–Field Interacting Particle System

Consider a system of N d–dimensional mean–field interacting particles:
$\mathcal{X}^{\eta,N} = \left(X_t^{1,\eta,N}, \ldots, X_t^{N,\eta,N}\right)_{t \geqslant 0}$,

$$dX_t^{i,\eta,N} = \left(b_0\left(X_t^{i,\eta,N}\right) + b_1\left(X_t^{i,\eta,N}, \rho_t^{\eta,N}\right) + \eta F\left(X_t^{i,\eta,N}\right)\right) dt + \sqrt{\frac{2}{\beta}} dW_t^i$$

$$\rho_t^{\eta,N} = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_t^{i,\eta,N}}$$

Make standard assumptions: Lipschitzness, F bounded, b_0 strongly contractive (at infinity), small interactions (b_1 small), ...

Consider observables of form: integral of a $R : \mathbb{R}^d \to \mathbb{R}$ wrt $\rho^{\eta,N}$

$$\left\langle \rho_t^{\eta,N}, R \right\rangle := \int_{\mathbb{R}^d} R \, d\rho_t^{\eta,N} = \frac{1}{N} \sum_{i=1}^{N} R\left(X_t^{i,\eta,N}\right)$$

Thévenin McKean–Vlasov Dynamics

Under our assumptions, propagation of chaos (uniform in $t \geqslant 0$ and η) to

$$
\begin{aligned}
d\widetilde{X}_t^\eta &= \left(b_0\left(\widetilde{X}_t^\eta\right) + b_1\left(\widetilde{X}_t^\eta, \xi_t^\eta\right) + \eta F\left(X_t^\eta\right)\right) dt + \sqrt{\frac{2}{\beta}} dW_t \\
\xi_t^\eta &= \mathrm{Law}\left(\widetilde{X}_t^\eta\right)
\end{aligned}
$$

with invariant measure $\widetilde{\nu}_\eta$ and generator $\mathcal{L}_\eta[\mu] = \mathcal{L}_0[\mu] + \eta\widetilde{\mathcal{L}}$

$$
\mathcal{L}_0\left[\mu\right] f = \left(b_0(x) + b_1\left(x,\mu\right)\right) \cdot \nabla f(x) + \frac{1}{\beta}\Delta f(x), \quad \widetilde{\mathcal{L}} f(x) = F(x) \cdot \nabla f(x)
$$

Standard consequences: Convergence of k–marginals of invariant measures of mean–field system to $\widetilde{\nu}_\eta^{\otimes k}$, for $\phi : \mathbb{R}^d \to \mathbb{R}$ Lipschitz

$$
\left\langle \rho_t^{\eta,N}, \phi \right\rangle \xrightarrow{N\to\infty} \left\langle \xi_t^\eta, \phi \right\rangle,
$$

etc.

Norton Mean–Field Interacting Particle System

N d–dimensional mean–field interacting particles
$\mathcal{Y}^{r,N} = \left(Y_t^{1,r,N}, \ldots, Y_t^{N,r,N}\right)_{t \geqslant 0}$ constrainted to

$$\Sigma_r^N := \left\{ x \in \left(\mathbb{R}^d\right)^N : \frac{1}{N} \sum_{i=1}^N R(x^i) = r \right\}$$

$$\begin{cases} dY_t^{1,r,N} = \left(b_0\left(Y_t^{i,r,N}\right) + b_1\left(Y_t^{i,r,N}, \varrho_t^{r,N}\right)\right) dt + \sqrt{\frac{2}{\beta}} dW_t^i \\ \qquad\qquad + F\left(Y_t^{i,r,N}\right) d\Lambda_t^{r,N} \\ \varrho_t^{r,N} = \frac{1}{N} \sum_{i=1}^N \delta_{Y_t^{i,r,N}} \\ \Lambda^{r,N} \quad \mathbb{R}\text{–valued semi–martingale fixing } d\left\langle \varrho_t^{r,N}, R \right\rangle = 0 \end{cases}$$

Norton Mean–Field Interacting Particle System

Assumption

- *(Observable)* $R \in \mathcal{C}^2\left(\mathbb{R}^d\right)$ *and* $\nabla R, \nabla^2 R$ *bounded*
- *(Controllability) There exists* $\alpha > 0$ *such that*

$$F(x) \cdot \nabla R(x) \geqslant \alpha, \qquad \forall x \in \mathbb{R}^d$$

- *(Non–décollage) We have for any* $\mu \in \mathcal{P}_p\left(\mathbb{R}^d\right)$

$$\left| \int_{\mathbb{R}^d} \left(b_0(x) + b_1\left(x, \mu\right)\right) \cdot \nabla R(x) \mu(dx) \right| \leqslant \gamma \mu\left(|x|^p\right)^{1/p} + \Gamma,$$

with $\gamma \geqslant 0$ *small enough.*

Norton Mean–Field Interacting Particle System

Making ansatz

$$\Lambda_t^N = \int_0^t \widetilde{\lambda}_s^N ds + \widetilde{\Lambda}_t^N$$

and using $d\left\langle \varrho_t^N, R\right\rangle = 0$ and assumptions, we find explicit expressions:

$$\widetilde{\lambda}_t^N = \lambda^N\left(\varrho_t^N\right) := \lambda\left(\rho_t^N\right) + \frac{h\left(\varrho_t^N\right)}{N}, \qquad \lambda(\mu) := -\frac{\langle \mu, \mathcal{L}_0[\mu]R\rangle}{\left\langle \mu, \widetilde{\mathcal{L}}R\right\rangle},$$

avec h bornée et $\left[\widetilde{\Lambda}^N, \widetilde{\Lambda}^N\right]_t = \mathrm{O}\left(\frac{t}{N}\right)$.

Proposition

For $p > 1$, λ is of linear growth on $\mathcal{P}_p\left(\mathbb{R}^d\right)$ and "almost Lipschitz"

$$|\lambda(\mu) - \lambda(\nu)| \leqslant \left(L + \mathcal{C}_{p,p*}(\mu,\nu)\right)\mathcal{W}_p(\mu,\nu), \quad \forall \mu, \nu \in \mathcal{P}_p\left(\mathbb{R}^d\right)$$

Norton Mean–Field Interacting Particle System

$$
\begin{cases}
dY_t^{i,r,N} = \left(b_0\left(Y_t^{i,r,N}\right) + b_1\left(Y_t^{i,r,N}, \varrho_t^{r,N}\right) + \lambda^N\left(\varrho_t^{r,N}\right) F\left(Y_t^{i,r,N}\right)\right) dt \\
\qquad\qquad + \sqrt{\frac{2}{\beta}} dW_t^i + F\left(Y_t^{i,r,N}\right) d\widetilde{\Lambda}_t^{r,N} \\
\varrho_t^{r,N} = \frac{1}{N} \sum_{i=1}^{N} \delta_{Y_t^{i,r,N}}
\end{cases}
$$

Proposition

Above dynamics is well–posed for any $N \in \mathbb{N}^*$, i.e. unique strong solution. With exchangeable initial conditions, we have uniform in N moment bounds: for any $N \in \mathbb{N}$

$$
\max_{i \in \{1,\dots,N\}} \mathbb{E}\left[\left|Y_t^{i,r,N}\right|^n\right] \leqslant \left(\widetilde{S}_n + \frac{A_n}{N}\right)\left(1 + \mathbb{E}\left[\left|Y_0^{1,r,N}\right|^n\right]\right)
$$

Norton McKean–Vlasov Dynamics

Formal $N \to \infty$ limit:

$$\begin{cases} d\widetilde{Z}_t = \left(b_0\left(\widetilde{Z}_t\right) + b_1\left(\widetilde{Z}_t, \widetilde{\zeta}_t\right) + \lambda\left(\widetilde{\zeta}_t\right) F\left(\widetilde{Z}_t\right)\right) dt + \sqrt{\dfrac{2}{\beta}} dW_t \\ \quad \widetilde{\zeta}_t = \mathrm{Law}\left(\widetilde{Z}_t\right) \end{cases}$$

Formally λ ensures that $\left\langle \widetilde{\zeta}_t, R \right\rangle = \left\langle \widetilde{\zeta}_0, R \right\rangle$ for all $t \geqslant 0$

Does this dynamics even exist?: Due to non–Lipschitzness of λ, Picard iteration is not contractive!

Theorem

Strong existence and pathwise uniqueness hold for the above dynamics.

Idea of proof:[2] Moment estimates + Finding right subspace $\Longrightarrow$ Recover contractivity $\Longrightarrow$ Apply Banach's Fixed Point Theorem

[2] Compare to the weak existence and uniqueness of Gärtner (1988) *On the McKean–Vlasov Limit for Interacting Diffusions*

Equivalence of Ensembles and Propagation of Chaos

Equivalence of Ensembles

Definition

Let $\eta_\star > 0$ be such $r : \eta \mapsto \widetilde{\nu}_\eta(R)$ is invertible on $[-\eta_\star, \eta_\star]$. Equivalence of the Thévenin and Norton ensembles holds if for any $t \geqslant 0$, $\eta \in [-\eta_\star, \eta_\star]$, and $\phi : \mathbb{R}^d \to \mathbb{R}$ Lipschitz

$$\left| \left\langle \rho_t^{\eta,N}, \phi \right\rangle - \left\langle \varrho_t^{r(\eta),N}, \phi \right\rangle \right| \to 0$$

in probability/L^p. Uniform equivalence holds convergence is uniform in $t \geqslant 0$ and $[-\eta_\star, \eta_\star]$.

Compare this to the definition (implicitly) used by Evans[3]:
For any extensive observable A

$$\langle A \rangle_{\text{Thévenin},N} - \langle A \rangle_{\mathrm{Norton},N} = \mathrm{O}_N(1)$$

[3] Evans (1993) *The equivalence of Norton and Thévenin ensembles*

Three useful observations

$$\lambda\left(\tilde{\nu}_\eta\right) = -\frac{\left\langle \tilde{\nu}_\eta, \mathcal{L}_0[\tilde{\nu}_\eta] R \right\rangle}{\left\langle \tilde{\nu}_\eta, \tilde{\mathcal{L}} R \right\rangle} = -\cancelto{0}{\frac{\left\langle \tilde{\nu}_\eta, \mathcal{L}_0[\tilde{\nu}_\eta] R \right\rangle}{\left\langle \tilde{\nu}_\eta, \tilde{\mathcal{L}} R \right\rangle}} + \eta$$

Consequence if $\tilde{Z}_0 \sim \tilde{\nu}_\eta$ then $\left(\tilde{Z}, \tilde{\zeta}\right) \overset{\mathrm{Law}}{=} \left(\tilde{X}^\eta, \xi^\eta\right)$ started at $\tilde{\nu}_\eta$.

For any $\phi : \mathbb{R}^d \to \mathbb{R}$

$$\left| \left\langle \rho_t^{\eta,N}, \phi \right\rangle - \left\langle \varrho_t^{r(\eta),N}, \phi \right\rangle \right| \leqslant \left| \left\langle \rho_t^{\eta,N}, \phi \right\rangle - \left\langle \xi_t^{\eta}, \phi \right\rangle \right| + \left| \left\langle \zeta_t^{r(\eta)}, \phi \right\rangle - \left\langle \varrho_t^{r(\eta),N}, \phi \right\rangle \right|,$$

where $\zeta^{r(\eta)}$ is the law of $\tilde{Z}$ started at $\tilde{\nu}_\eta$.

For any $\phi : \mathbb{R}^d \to \mathbb{R}$ Lipschitz

$$\mathbb{E}\left[\left| \left\langle \zeta_t^{r(\eta)}, \phi \right\rangle - \left\langle \varrho_t^{r(\eta),N}, \phi \right\rangle \right| \right] \leqslant \|\phi\|_{\mathrm{Lip}}\, \mathbb{E}\left[\mathcal{W}_1\left(\zeta_t^{r(\eta)}, \varrho_t^{r(\eta),N} \right) \right]$$

Punchline: *(Quantitative/uniform) PoC* $\Longrightarrow$ *(quantitative/uniform)* EoE

Qualitative Propagation of Chaos

It remains to show: *If* $\varrho_0^N \to \widetilde{\zeta}_0$ *as* $N \to \infty$, *for any* $t \geqslant 0$ *does*

$$\varrho_t^N \to \widetilde{\zeta}_t, \qquad \text{as } N \to \infty?$$

Theorem

Propagation of chaos of mean–field Norton system towards McKean–Vlasov Norton system holds.

Idea of proof:

- Strong solution $\implies$ uniqueness of martingale problem
- Moment bounds $\implies$ tightness

Standard tightness–uniqueness argument[4]

[4] See for example: Méléard (1996) *Asymptotic Behaviour of some interacting particle systems; McKean-Vlasov and Boltzmann models*

Quantitative Propagation of Chaos

Non–Lipschitzness of λ makes using synchronous coupling à la Sznitman[5]/Malrieu[6] difficult.

Solution: Stability estimates inspired by[7]

Proposition

Assume $\widetilde{\zeta}_0$ has enough moments. There exists $C > 0$ such that $\forall \mu \in \mathcal{P}_p\left(\mathbb{R}^d\right)$

$$\left|\lambda\left(\widetilde{\zeta}_t\right) - \lambda(\mu)\right| \leqslant C\mathcal{W}_p\left(\widetilde{\zeta}_t, \mu\right)$$

Finite–time quantitative propagation of chaos now easy.

Reminder: $p > 1$

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[5] Sznitman (1989) *Topics in the propagation of chaos*

[6] Malrieu (2001) *Logarithmic Sobolev inequalities for some nonlinear PDE's*

[7] Gerber Hoffmann Vaes (2023) *Mean-field limits for Consensus-Based Optimization and Sampling*

Quantitative Propagation of Chaos

Under very strong (irrealistic) hypotheses (global strong contractivity, very weak interactions, assumptions on R and F, ...), uniform propagation of chaos is provable!

Theorem

Under very strong assumptions and assuming $\varrho_0^N \to \widetilde{\zeta}_0$ fast enough, uniform in time propagation of chaos holds: for any $n \geqslant p$

$$\sup_{t \geqslant 0} \mathbb{E}\left[\mathcal{W}_n^n\left(\widetilde{\zeta}_t, \varrho_t^N\right)\right] \leqslant C N^{-\min\{1/2, n/d\}}$$

λ is "almost Lipschitz" only for $p > 1$ is a technical obstacle to using reflection coupling à la Eberle[8]

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[8] Durmus Eberle Guillin Zimmer *An elementary approach to uniform in time propagation of chaos*

Some Extensions and Perspectives

- Many interesting objects worth studying in Norton dynamics
  - Norton McKean–Vlasov dynamics: Non–linear Markov process with an oblique constraint on law

$$d\widetilde{Z}_t = \left(b_0\left(\widetilde{Z}_t\right) + b_1\left(\widetilde{Z}_t, \widetilde{\zeta}_t\right) + \lambda\left(\widetilde{\zeta}_t\right)F\left(\widetilde{Z}_t\right)\right)dt + \sqrt{\frac{2}{\beta}}dW_t$$

  - Fluctuations? PoC does not see Martingale $\widetilde{\Lambda}^N$, but fluctuations do
- Current hypotheses are very strong (unrealistic)
  - Extension to irregular coefficients to weaken controlability assumption
  - Reflection coupling to weaken global contractivity
  - Other models: kinetic Langevin (on torus). Atom chains?
  - Non–linear dynamics with multiple invariant measures and "local uniform PoC".
- Original motivation: Computing transport coefficients
  - Performance of estimator:

$$\frac{r}{\int_0^T \lambda_t\left(\varrho_t^{r,N}\right)dt} \xrightarrow{N,T\to\infty,r\to 0} \rho$$

An idea to make reflection coupling work

Inspired by[9] we could study the invariant measures of a one–dimensional sticky non–linear SDE:

$$dr_t = \left(\kappa_{\eta_\star}(r_t)r_t + L_{b,2}\mathbb{E}\left[r_t^p\right]^{1/p}\right)dt + 2\sqrt{\frac{2}{\beta}}\mathbf{1}_{\{r_t>0\}}dB_t$$

δ_0 is an invariant measure of the above dynamics. When is it the only one? Exponential ergodicity?

Bounding process $\left|\widetilde{Z}_t^{i,r} - Y_t^{i,r,N}\right| \leqslant r_t^{i,\delta,N}$,

$$dr_t^{i,\delta,N} = \left(\kappa_{\eta_\star}\left(r_t^{i,\delta,N}\right)r_t^{i,\delta,N} + \left(\sum_{i=1}^{N}\left(r_t^{i,\delta,N}\right)^p\right)^{1/p}\right)dt$$
$$+ 2\sqrt{\frac{2}{\beta}}\phi_{\mathrm{rc}}^{\delta}\left(r_t^{i,r,N}\right)dB_t^i$$

[9] Durmus Eberle Guillin Schuh (2022) *Sticky non–linear SDEs and convergence of McKean–Vlasov without confinement*

An idea about the Fluctuations

$$\widetilde{\Lambda}_t^N = -\sqrt{\frac{2}{\beta}} \int_0^t \frac{\frac{1}{N}\sum_{i=1}^N \nabla R\left(Y_s^{i,N}\right) \cdot dW_s}{\left\langle \varrho_s^N, \widetilde{\mathcal{L}} R \right\rangle}$$

Naive formal limit

$$\text{“}\frac{1}{\sqrt{N}} \sum_{i=1}^N \left(\sqrt{\frac{2}{\beta}} W_t^i - \int_0^t F\left(Y_s^{i,N}\right) d\widetilde{\Lambda}_s \right)$$

$$\to \sqrt{\frac{2}{\beta}} \int_0^t \left[\int_{\mathbb{R}^d} \dot{W}(s,x)dx - \frac{\int_{\mathbb{R}^d} F(z)\nabla R(z) \cdot \dot{W}(s,x) \widetilde{\zeta}_s(dz)}{\left\langle \widetilde{\zeta}_s, \widetilde{\mathcal{L}} R \right\rangle} \right] ds,\text{”}$$

with $\dot{W}$ a space–time white noise.

Fluctuations also obliquely constrained?

Norton kinetic Langevin on torus

$$\left(q_t^{1,N}, p_t^{1,N}, \ldots, q_t^{N,N}, p_t^{N,N}\right) \in \left(\mathbb{T}^d \times \mathbb{R}^d\right)^N$$

$$\begin{aligned} dq_t^{i,N} &= p_t^{i,N} dt \\ dp_t^{i,N} &= -\left(\nabla U(q_t^{i,N}) + \frac{1}{N}\sum_{i=1}^{N} \nabla W\left(q_t^{i,N} - q_t^{j,N}\right)\right) dt - \gamma p_t^{i,N} dt \\ &\qquad + \sqrt{\frac{2\gamma}{\beta}} dW_t^i + F\left(q_t^{i,N}, p_t^{i,N}\right) d\Lambda_t^N \end{aligned}$$

The homologue of λ is $\mathcal{W}_1$ Lipschitz!

Mobility $R(q,p) = u^\top p$ with $u \in \mathbb{S}^{d-1}$ and $F(q,p) \equiv F \in \mathbb{S}^{d-1}$ trivial satisfies controlability assumption if $u \cdot F \neq 0$.

Noé's class of observables work well to $R(q,p) = G(q) \cdot p$ with $G : \mathbb{R}^d \to \mathbb{R}^d$